

CRYSTAL STRUCTURES AND LATTICE PARAMETERS OF ALLOTROPES OF THE ELEMENTS

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The crystal structures of the allotropic forms of the elements are presented in terms of the Pearson symbol, the Strukturbericht designation, and the prototype of the structure. The temperatures of the phase transformations are listed in degrees Celsius and the pressures are in the Gpa. A consistent nomenclature is used, whereby all allotropes are labeled by Greek letters. The lattice parameters of the units cells are given in nanometers (nm) and are considered to be accurate to ± 2 in the last reported digit.

This compilation is restricted to changes in crystal structures that occur as a result of a change in temperature or pressure. Low-

temperature structures are included for the diatomic and rare gases, which show many similarities with respect to the metallic elements. The elements identified with an asterisk (*) have polymorphic structures based on different molecular configurations. The crystal data given for these elements refer to the most stable structure at room temperature.

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Element	Temper- ature, °C	Pressure, GPa	Pearson symbol	Space group	Struktur- bericht designation	Prototype	Lattice parameters, nm			Comment, c/a or α or β
							a	b	c	
Ac	25	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.5311
Ag	25	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.40857
α Al	25	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.40496
β Al	25	>20.5	$hP2$	$P6_3/mmc$	A3	Mg	0.2693	...	0.4398	1.6331
α' Am	25	atm	$hP4$	$P6_3/mmc$	A3'	α La	0.34681	...	1.1241	2*1.621
α Am	>769	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.4894
β Am	>1074	atm	$cI2$	$Im\bar{3}m$	A2	W	?
γ Am	25	>15	$oC4$	$Cmcm$	A20	α U	0.3063	0.5968	0.5169	...
α Ar	<-189.35	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.5316
(β Ar)	<-189.40	atm	$hP2$	$P6_3/mmc$	A3	Mg	0.3760	...	0.6141	1.633
α As	25	atm	$hR2$	$R\bar{3}m$	A7	α As	0.41319	$\alpha = 54.12^\circ$
eAs	>448	atm	$oC8$	$Cmca$...	P(black)	0.362	1.085	0.448	...
Au	25	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.40782
β B	25	atm	$hR105$	$R\bar{3}m$...	β B	1.017	$\alpha = 65.12^\circ$
α Ba	25	atm	$cI2$	$Im\bar{3}m$	A2	W	0.50227
β Ba	25	>5.33	$hP2$	$P6_3/mmc$	A3	Mg	0.3901	...	0.6154	1.5775
γ Ba	25	>23	?	?
α Be	25	atm	$hP2$	$P6_3/mmc$	A3	Mg	0.22859	...	0.35845	1.5681
β Be	>1270	atm	$cI2$	$Im\bar{3}m$	A2	W	0.25515
γ Be	25	>9.3	?
α Bi	25	atm	$hR2$	$r\bar{3}m$	A7	α As	0.47460	$\alpha = 57.23^\circ$
β Bi	25	>2.6	$mC4$	$C2/m$...	β Bi	0.6674	0.6117	0.3304	$\beta = 110.33^\circ$
γ Bi	25	>3.0	$mp3$?	0.605	0.42	0.465	$\beta = 85.33^\circ$
σ Bi	25	>4.3	?	?
eBi	25	>6.5	?	?
ζ Bi	25	>9.0	$cI2$	$Im\bar{3}m$	A2	W	0.3800
α Bk	25	atm	$hP4$	$P6_3/mmc$	A3'	α La	0.3416	...	1.1069	2*1.620
β Bk	>977	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.4997
Br	<7.25	atm	$oC8$	$Cmca$...	Cl	0.668	0.449	0.874	...
C	25	atm	$hP4$	$P6_3/mmc$	A9	C(graphite)	0.24612	...	0.6709	2.7258
(graphite)										
C (diamond)	25	>60	$cF8$	$Fd\bar{3}m$	A4	C(diamond)	0.35669
C (hd)	25	HP	$hP4$	$P6_3/mmc$...	C (hd)	0.2522	...	0.4119	1.633
α Ca	25	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.55884
β Ca	>443	atm	$cI2$	$Im\bar{3}m$	A2	W	0.4480
γ Ca	25	>1.5	?
Cd	25	atm	$hP2$	$P6_3/mmc$	A3	Mg	0.29793	...	0.56196	1.8862
α Ce	<-177	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.485
β Ce	25	atm	$hP4$	$P6_3/mmc$	A3'	α La	0.36810	...	1.1857	2*1.611
γ Ce	25	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.51610
δ -Ce	>726	atm	$cI2$	$Im\bar{3}m$	A2	W	0.412
α' Ce	25	>5.4	$oC4$	$Cmcm$	A20	α U	0.3049	0.5998	0.5215	...

Element	Temperature, °C	Pressure, GPa	Pearson symbol	Space group	Struktur- bericht designation	Prototype	Lattice parameters, nm			Comment, c/a or α or β
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α Cf	25	atm	$hP4$	$P6_3/mmc$	$A3'$	α La	0.339	...	1.1015	2*1.625
β Cf	>590	atm	$cF4$	$Fm\bar{3}m$	$A1$	Cu	?
Cl	<-102	atm	$oC8$	$Cmca$...	Cl	0.624	0.448	0.826	...
α Cm	25	atm	$hP4$	$P6_3/mmc$	$A3'$	α La	0.3496	...	1.1331	2*1.621
β Cm	>1277	atm	$cF4$	$Fm\bar{3}m$	$A1$	Cu	0.4382
ϵ Co	25	atm	$hP2$	$P6_3/mmc$	$A3$	Mg	0.25071	...	0.40686	1.6228
α Co	>422	atm	$cF4$	$Fm\bar{3}m$	$A1$	Cu	0.35447
α Cr	25	atm	$cI2$	$I\bar{m}3m$	$A2$	W	0.28848
α' Cr	25	HP	$tI2$	$I4/mmm$...	α' Cr	0.2882	...	0.2887	1.002
α Cs	25	atm	$cI2$	$I\bar{m}3m$	$A2$	W	0.6141
β Cs	25	>2.37	$cF4$	$Fm\bar{3}m$	$A1$	Cu	0.6465
β' Cs	25	>4.22	$cF4$	$Fm\bar{3}m$	$A1$	Cu	0.5800
γ Cs	25	>4.27	?
Cu	25	atm	$cF4$	$Fm\bar{3}m$	$A1$	Cu	0.36146
α Dy	<-187	atm	$oC4$	$Cmcm$...	α' Dy	0.3595	0.6184	0.5678	...
α Dy	25	atm	$hP2$	$P6_3/mmc$	$A3$	Mg	0.35915	...	0.56501	1.5732
β Dy	>1381	atm	$cI2$	$I\bar{m}3m$	$A2$	W	0.403
γ Dy	25	>7.5	$hR3$	$R\bar{3}m$...	α Sm	0.3436	...	2.483	4.5*1.606
Er	25	atm	$hP2$	$P6_3/mmc$	$A3$	Mg	0.35592	...	0.55850	1.5692
α Es	25	atm	$hP4$	$P6_3/mmc$	$A3'$	α La	?
β Es	?	atm	$cF4$	$Fm\bar{3}m$	$A1$	Cu	?
Eu	25	atm	$cI2$	$I\bar{m}3m$	$A2$	W	0.45827
α F	<-227.6	atm	$mC8$	$C2/c$...	α F	0.550	0.338	0.728	$\beta = 102.17^\circ$
β F	<-219.67	atm	$cP16$	$Pm\bar{3}n$...	γ O	0.667
α Fe	25	atm	$cI2$	$I\bar{m}3m$	$A2$	W	0.28665
γ Fe	>912	atm	$cF4$	$Fm\bar{3}m$	$A1$	Cu	0.36467
σ Fe	>1394	atm	$cI2$	$I\bar{m}3m$	$A2$	W	0.29315
ϵ Fe	25	>13	$hP2$	$P6_3/mmc$	$A3$	Mg	0.2468	...	0.396	1.603
α Ga	25	atm	$oC8$	$Cmca$	$A11$	α Ga	0.45186	0.76570	0.45258	...
β Ga	25	>1.2	$tI2$	$I4/mmm$	$A6$	In	0.2808	...	0.4458	1.588
γ Ga	-53	>3.0	$oC40$	$Cmcm$...	γ Ga	1.0593	1.3523	0.5203	...
α Gd	25	atm	$hP2$	$P6_3/mmc$	$A3$	Mg	0.36336	...	0.57810	0.5910
β Gd	>1235	atm	$cI2$	$I\bar{m}3m$	$A2$	W	0.406
γ Gd	25	>3.0	$hR3$	$R\bar{3}m$...	α Sm	0.361	...	2.603	4*1.60
α Ge	25	atm	$cF8$	$Fd\bar{3}m$	$A4$	C (diamond)	0.56574
β Ge	25	>12	$tI4$	$I4/\bar{a}md$	$A5$		β Sn	0.4884	...	0.2692
γ Ge	25	>12->atm	$tP12$	$P4_2\bar{2}_2$...	σ Ge	0.593	...	0.698	1.18
σ Ge	LT	>12	$cII6$	$I\bar{m}3m$...	γ Si	0.692
α H	<-271.9	atm	$cF4$	$Fm\bar{3}m$	$A1$	Cu	0.5338
β H	<-259.34	atm	$hP2$	$P6_3/mmc$	$A3$	Mg	0.3776	...	0.6162	1.632
α He	<-268.94	atm	$hP2$	$P6_3/mmc$	$A3$	Mg	0.3555	...	0.5798	1.631
β He	>258	0.125	$cF4$	$Fm\bar{3}m$	$A1$	Cu	0.4240
γ He	<-271.47	0.03	$cI2$	$I\bar{m}3m$	$A2$	W	0.4110
α Hf	25	atm	$hP2$	$P6_3/mmc$	$A3$	Mg	0.31946	...	0.50510	1.5811
β Hf	>1995	atm	$cI2$	$I\bar{m}3m$	$A2$	W	0.3610
α Hg	<-38.84	atm	$hR1$	$R\bar{3}m$	$A10$	α Hg	0.3005	$\alpha = 70.53^\circ$
β Hg	<-194	HP	$tI2$	$I4/mmm$...	β Hg	0.3995	...	0.2825	0.707
γ Hg	<-194	c.w.	$hR1$?
α Ho	25	atm	$hP2$	$P6_3/mmc$	$A3$	Mg	0.35778	...	0.56178	1.5702
β Ho	25	>7.5	$hR3$	$R\bar{3}m$...	α Sm	0.334	...	2.45	4.5*1.63
I	25	atm	$oC8$	$Cmca$...	Cl	0.72697	0.47903	0.97942	...
In	25	atm	$tI2$	$I4/mmm$	$A6$	In	0.3253	...	0.49470	1.5210
Ir	25	atm	$cF4$	$Fm\bar{3}m$	$A1$	Cu	0.38392
K	25	atm	$cI2$	$I\bar{m}3m$	$A2$	W	0.5321
Kr	<-157.39	atm	$cF4$	$Fm\bar{3}m$	$A1$	Cu	0.5810
α La	25	atm	$hP4$	$P6_3/mmc$	$A3'$	α La	0.37740	...	1.2171	2*1.6125
β La	>310	atm	$cF4$	$Fm\bar{3}m$	$A1$	Cu	0.5303
γ La	>865	atm	$cI2$	$I\bar{m}3m$	$A2$	W	0.426
β' La	25	>2.0	$cF4$	$Fm\bar{3}m$	$A1$	Cu	0.517
α Li	<-193	atm	$hP2$	$P6_3/mmc$	$A3$	Mg	0.3111	...	0.5093	1.637

Element	Temper- ature, °C	Pressure, GPa	Pearson symbol	Space group	Struktur- bericht designation	Prototype	Lattice parameters, nm			Comment, c/a or α or β
							a	b	c	
βLi	25	atm	$cI2$	$Im\bar{3}m$	A2	W	0.35093
γLi	<-201	c.w.	$cF4$	$Fm\bar{3}m$	A1	Cu	0.4388
Lu	25	atm	$hP2$	$P\bar{6}_3/mmc$	A3	Mg	0.35052	...	0.55494	1.5832
Mg	25	atm	$hP2$	$P\bar{6}_3/mmc$	A3	Mg	0.32094	...	0.52107	1.6236
αMn	25	atm	cl58	$I\bar{4}\bar{3}m$	A12	αMn	0.89126
βMn	>710	atm	$cP20$	$P4_{1}32$	A13	βMn	0.63152
γMn	>1079	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.3860
σMn	>1143	atm	$cI2$	$Im\bar{3}m$	A2	W	0.3080
Mo	25	atm	$cI2$	$Im\bar{3}m$	A2	W	0.31470
αN	<-237.6	atm	$cP8$	$Pa\bar{3}$...	αN	0.5661
βN	<-210.00	atm	$hP4$	$P\bar{6}_3/mmc$...	βN	0.4050	...	0.6604	1.631
γN	<-253	>3.3	$tP4$	$P4_{1}/mm$...	γN	0.3957	...	0.5109	1.291
αNa	<-233	atm	$hP2$	$P\bar{6}_3/mmc$	A3	Mg	0.3767	...	0.6154	1.634
βNa	25	atm	$cI2$	$Im\bar{3}m$	A2	W	0.42906
Nb	25	atm	$cI2$	$Im\bar{3}m$	A2	W	0.33004
αNd	25	atm	$hP4$	$P\bar{6}_3/mmc$	A3'	αLa	0.36582	...	1.17966	2*1.6124
βNd	>863	atm	$cI2$	$Im\bar{3}m$	A2	W	0.413
γNd	25	>5.0	$cF4$	$Fm\bar{3}m$	A1	Cu	0.480
Ne	<-243.59	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.4462
Ni	25	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.35240
αNp	25	atm	$oP8$	$Pnma$	A_c	αNp	0.6663	0.4723	0.4887	...
βNp	>280	atm	$tP4$	$P4_{2}2$	A_d	βNp	0.4883	...	0.3389	0.694
γNp	>576	atm	$cI2$	$Im\bar{3}m$	A2	W	0.352
αO	<-243.3	atm	$mC4$	$C\bar{2}m$...	αO	0.5403	0.3429	0.5086	$\beta = 132.53^\circ$
βO	<-229.6	atm	$hR2$	$R\bar{3}m$...	βO	0.4210	$\alpha = 46.27^\circ$
γO	<-218.79	atm	$cP16$	$Pm\bar{3}n$...	γO	0.683
Os	25	atm	$hP2$	$P\bar{6}_3/mmc$	A3	Mg	0.27341	...	0.43918	1.6063
P (black)	25	atm	$oC8$	$Cmca$...	P (black)	0.33136	1.0478	0.43763	...
αPa	25	atm	$tI2$	$I\bar{4}/mmm$	A_a	αPa	0.3921	...	0.3235	0.825
βPa	>1170	atm	$cI2$	$Im\bar{3}m$	A2	W	0.381
αPb	25	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.49502
βPb	25	>10.3	$hP2$	$P\bar{6}_3/mmc$	A3	Mg	0.3265	...	0.5387	1.650
Pd	25	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.38903
αPm	25	atm	$hP4$	$P\bar{6}_3/mmc$	A3'	αLa	0.365	...	1.165	2*1.60
βPm	>890	atm	$cI2$	$Im\bar{3}m$	A2	W	(0.410)
αPo	25	atm	$cP1$	$Pm\bar{3}m$	A_h	αPo	0.3366
βPo	>54	atm	$hR1$	$R\bar{3}m$...	βPo	0.3373	$\alpha = 98.08^\circ$
αPr	25	atm	$hP4$	$P\bar{6}_3/mmc$	A3'	αLa	0.36721	...	1.18326	2*1.6111
βPr	>795	atm	$cI2$	$Im\bar{3}m$	A2	W	0.413
γPr	25	>4.0	$cF4$	$Fm\bar{3}m$	A1	Cu	0.488
Pt	25	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.39236
αPu	25	atm	$mP16$	$P2_{1}/m$...	αPu	0.6183	0.4822	1.0963	$\beta = 101.97^\circ$
βPu	>125	atm	$mI34$	$I\bar{2}/m$...	βPu	0.9284	1.0463	0.7859	$\beta = 92.13^\circ$
γPu	>215	atm	$oF8$	$Fddd$...	γPu	0.31587	0.57682	1.0162	...
σPu	>320	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.46371
$\sigma'\text{Pu}$	>463	atm	$tI2$	$I\bar{4}/mmm$	A6	In	0.33261	...	0.44630	1.3418
ePu	>483	atm	$cI2$	$Im\bar{3}m$	A2	W	0.36343
Ra	25	atm	$cI2$	$Im\bar{3}m$	A2	W	0.5148
αRb	25	atm	$cI2$	$Im\bar{3}m$	A2	W	0.5705
βRb	25	>1.08	?
γRb	25	>2.05	?
Re	25	atm	$hP2$	$P\bar{6}_3/mmc$	A3	Mg	0.27609	...	0.4458	1.6145
Rh	25	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.38032
Ru	25	atm	$hP2$	$P\bar{6}_3/mmc$	A3	Mg	0.27058	...	0.42816	1.5824
αS	25	atm	$oFI28$	$Fddd$	A16	αS	1.0464	1.28660	2.44860	...
αSb	25	atm	$hR2$	$R\bar{3}m$	A7	αAs	0.45067	$\alpha = 57.11^\circ$
βSb	25	>5.0	$cP1$	$Pm\bar{3}m$	A_h	αPo	0.2992
γSb	25	>7.5	$hP2$	$P\bar{6}_3/mmc$	A3	Mg	0.3376	...	0.5341	1.582
σSb	25	>14.0	$mp3$?	0.556	0.404	0.422	$\beta = 86.0^\circ$
αSc	25	atm	$hP2$	$P\bar{6}_3/mm$	A3	Mg	0.33088	...	0.52680	1.5921

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βSc	>1337	atm	$cI2$	$Im\bar{3}m$	A2	W	(0.373)
γSe	25	atm	$hP3$	$P\bar{3}_121$	A8	γSe	0.43659	...	0.49537	1.1346
αSi	25	atm	$cF8$	$Fd\bar{3}m$	A4	C (diamond)	0.54306
βSi	25	>9.5	$tI4$	$I4/amd$	A5		0.4686	...	0.2585	0.552
γSi	25	>16.0	$cI16$	$Im\bar{3}m$...	γSi	0.6636
σSi	25	>16→atm	$hP4$	$P6_3/mmc$	A3'	αLa	0.380	...	0.628	1.653
αSm	25	atm	$hR3$	$R\bar{3}m$...	αSm	0.36290	...	2.6207	4*1.6048
βSm	>734	atm	$hP2$	$P6_3/mmc$	A3	Mg	0.36630	...	0.58448	1.5956
$\gamma'\text{Sm}$	>922	atm	$cI2$	$Im\bar{3}m$	A2	W	(0.410)
σSm	25	>4.0	$hP4$	$P6_3/mmc$	A3'	αLa	0.3618	...	1.166	2*1.611
αSn	<13	atm	$cF8$	$Fd\bar{3}m$	A4	C (diamond)	0.64892
βSn	25	atm	$tI4$	$I4/amd$	A5		0.58318	...	0.31818	0.5456
γSn	25	>9.0	$tI2$?	...	γSn	0.370	...	0.337	0.91
αSr	25	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.6084
βSr	>547	atm	$cI2$	$Im\bar{3}m$	A2	W	0.487
$\beta'\text{Sr}$	25	>3.5	$cI2$	$Im\bar{3}m$	A2	W	0.4437
Ta	25	atm	$cI2$	$Im\bar{3}m$	A2	W	0.33030
$\alpha'\text{Tb}$	<-53	atm	$oC4$	$Cmcm$...	$\alpha'\text{Dy}$	0.3605	0.6244	0.5706	...
aTb	25	atm	$hP2$	$P6_3/mmc$	A3	Mg	0.36055	...	0.56966	1.5800
βTb	>1289	atm	$cI2$	$Im\bar{3}m$	A2	W	(0.407)
γTb	25	>6.0	$hR3$	$R\bar{3}m$...	αSm	0.341	...	2.45	4*1.60
Tc	25	atm	$hP2$	$P6_3/mmc$	A3	Mg	0.2738	...	0.4393	1.604
αTe	25	atm	$hP3$	$P\bar{3}_121$	A8	γSe	0.44566	...	0.59264	1.3298
βTe	25	>2.0	$hR2$	$R\bar{3}m$	A7	αAs	0.469	$\alpha = 53.30^\circ$
γTe	25	>7.0	$hR1$	$R\bar{3}m$...	βPo	0.3002	$\alpha = 103.3^\circ$
αTh	25	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.50842
βTh	>1360	atm	$cI2$	$Im\bar{3}m$	A2	W	0.411
αTi	25	atm	$hP2$	$P6_3/mmc$	A3	Mg	0.29506	...	0.46835	1.59873
βTi	>882	atm	$cI2$	$Im\bar{3}m$	A2	W	0.33065
ωTi	25	HP→atm	$hP3$	$P6/mmm$...	ωTi	0.4625	...	0.2813	0.6082
αTl	25	atm	$hP2$	$P6_3/mmc$	A3	Mg	0.34566	...	0.55248	1.5983
βTl	>230	atm	$cI2$	$Im\bar{3}m$	A2	W	0.3879
γTl	25	HP	$cF4$	$Fm\bar{3}m$	A1	Cu	?
Tm	25	atm	$hP2$	$P6_3/mmc$	A3	Mg	0.35375	...	0.55540	1.5700
αU	25	atm	$oC4$	$Cmcm$	A20	αU	0.28537	0.58695	0.49548	...
βU	>668	atm	$tP30$	$P4_2/mnm$	A_b	βU	1.0759	...	0.5656	0.526
γU	>776	atm	$cI2$	$Im\bar{3}m$	A2	W	0.3524
V	25	atm	$cI2$	$Im\bar{3}m$	A2	W	0.30240
W	25	atm	$cI2$	$Im\bar{3}m$	A2	W	0.31652
Xe	<-111.76	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.6350
αY	25	atm	$hP2$	$P6_3/mmc$	A3	Mg	0.36482	...	0.57318	1.5711
βY	>1478	atm	$cI2$	$Im\bar{3}m$	A2	W	(0.410)
αYb	<-3	atm	$hP2$	$P6_3/mmc$	A3	Mg	0.38799	...	0.63859	1.6459
βYb	25	atm	$cF4$	$Fm\bar{3}m$	A1	Cu	0.54848
γYb	>795	atm	$cI2$	$Im\bar{3}m$	A2	W	0.444
Zn	25	atm	$hP2$	$P6_3/mmc$	A3	Mg	0.26650	...	0.49470	1.8563
αZr	25	atm	$hP2$	$P6_3/mmc$	A3	Mg	0.32316	...	0.51475	1.5929
βZr	>863	atm	$cI2$	$Im\bar{3}m$	A2	W	0.36090
ωZr	25	HP→atm	$hP2$	$P6/mmm$...	ωTi	0.5036	...	0.3109	0.617